INSTITUTE OF NATURAL AND APPLIED SCIENCES
UNIVERSITY OF ÇUKUROVA

MSc THESIS

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DIRAC EQUATION AND HYDROGEN ATOM

DEPARTMENT OF PHYSICS

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We certify that this thesis is satisfactory for the award of master of science degree

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ABSTRACT

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According to the Theory of Special Relativity laws of physics valid in one inertial frame are valid in other inertial frames. Also,the speed of light is invariant under Lorentz transformations. From these principles we try to obtain a relativistic quantum theory which also agrees with the principles of non-relativistic quantum theory. This was achieved by Dirac who found an equation which gives antiparticle solutions as well as solutions for particle with spin 1/2 .

On the other hand, in Dirac equation odd operators couple small and large components of the wave function. In order to decouple them Foldy-wouthuysen transformations are used.

In this thesis we applied the methods of Relativistic Quantum mechanics and Foldy-wouthuysen transformations to the hydrogen and investigated the corrections brought to the energy levels by a relativistic hamiltonian.

Key Words: Klein-Gordon equation, Dirac equation, Dirac matrices, Foldy-Wouthuysen transformations, the hydrogen atom.

ÖZ

YÜKSEK LİSANS TEZİ

Dirac Denklemi ve Hidrojen Atomu

Hasan ARSLAN

ÇUKUROVA ÜNİVERSİTESİ
FEN BİLİMLERİ ENSTİTÜSÜ
FİZİK ANABİLİM DALI

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Özel görelilik kuramına göre eylemsiz bir çerçevede geçerli olan fizik yasaları başka eylemsiz çerçevede de geçerlidir. Ayrıca ışık hızı Lorentz dönüşümleri altında değişmezdir. Buna dayanarak görelilikli olmayan kuantum mekaniğinden görelikli olan kuantum mekaniğine geçiş yaparken görelilikli olmayan kuantum mekaniğinin kurallarının geçerlilikleri korunmalıdır. Bu geçişi gerçekleştiren Dirac, 1/2 spinli parçacığın yanısıra antiparçacığın çözümlerini de buldu.

Öte yandan Dirac denkleminde antiparçacığın çözümlerini veren küçük dalga fonksiyonu, 1/2 spinli parçacığın çözümlerini veren büyük dalga fonksiyonuyla tek (odd) operatörlerle ilişkilenir. Parçacık ve antiparçacık çözümlerinin birbirine karışmasını önlemek için Foldy-Wouthuysen dönüşümleri kullanılır.

Bu çalışmada bu yöntemler özetlenmiş ve hidrojen atomuna uygulanmıştır. Görelikli hamiltonyenin enerji düzeylerine getirdiği düzeltmeler incelenmiştir.

Anahtar kelimeler: Klein-Gordon denklemi, Dirac denklemi, Dirac matrisleri, Foldy-Wouthuysen dönüşümleri, Hidrojen atomu

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CONTENTS

CHAPTER 1

INTRODUCTION

1.1 Formulation of a Relativistic Quantum Theory

A real quantum theory should satisfy the principles of relativity theory, that is, laws of motion true in an inertial frame is valid in another inertial frame and speed of light is invariant under Lorentz transformation.

Relativistic quantum theory must agree with principles of nonrelativistic theory.These principles are;

1. For every physical system there is a wave function ψ which includes all information about the system that we can know. At time t for coordinates $(q_1 ... s_n)$ the wave function has a physical meaning only if $|\psi(q_1..., s_1...,t)|^2 \geq 0$. This representation $|\psi|^2$ of finding the particle with coordinates $q_1 ..., s_1 ... s_n$ at time t is the probability. The sum of positive contributions $|\psi|^2$ for all values of given coordinates $(q_1 ... q_n, s_1 ... s_n)$ must be finite for all acceptable wave functions;

2. A linear hermitian operator is used to represent a physical observable . For example, we use $p_i \rightarrow (\hbar / i)(\partial / \partial q_i)$ to represent momentum ,

3.When a physical observable represented by an operator Ω is measured for a physical system one obtains one of the eigenvalue ω_n which is real for a hermitian operator ,

$$\Omega \psi_n = \omega_n \psi_n$$

After the measurement, the system is left in the eigenstate ψ_n

4.According to expansion postulate a state function of a physical system can be written in terms of a complete orthonormal set of eigenfunctions ψ_n .That is ,

$$\psi=\sum a_n \psi_n$$

and

$$\sum\int(dq_1...)\ \psi_n{*}(q...,s...,t)\psi_m(q_1...,s...,t)=\delta_{nm}$$

is the statement of orthonormality .

ψ can be written as $|\psi>=\psi$, and $\psi^+=<\psi|$. Then ,

$$\psi\psi^+=<\psi|\psi>=<a_n\psi|a_m\psi>=a_na_m\delta_{nm}=|a_n|^2$$

records the probability that the system is in the nth eigenstate .

5.A physical observable Ω measures any one of its eigenvalues ω_n with a probability $|a_n|^2$. The average of physical observable measurement is given by $<\Omega>$

$$<\Omega>_\psi=\sum\int\psi{*}(q_1...,s...,t)\Omega\,\psi(q_1...,s...,t)(dq_1...)=\sum|a_n|^2\omega_n$$

6. The time dependence of a physical system is given by the Schröginger equation :

$$i\hbar\,(\partial\psi/\partial t)=H\psi$$

Hamiltonian H is a linear hermitian operator and has no explicit time dependence , i.e. $\partial H/\partial t=0$, for a closed physical system.

From linearity of H and conservation of probability we conclude that

$$(d/dt)\sum\int\psi{*}\psi(dq_1...)=i/\hbar\sum\int(dq_1...)[(H\psi)\psi{*}-\psi{*}(H\psi)]=0$$

Depending on these six principles of nonrelativistic theory we try to find the coresponding relativistic quantum theory.

1.2 Attempts to Relativistic Quantum Formulation

For an isolated free particle the nonrelativistic hamiltonian is

$$H=\frac{p^2}{2m} \tag{1.1}$$

In quantum mechanics we use the operators

$$H\rightarrow i\hbar\frac{\partial}{\partial t} \tag{1.2}$$

$$p \rightarrow \frac{\hbar}{i}\ \vec{\nabla} \tag{1.3}$$

Then the nonrelativistic Schrödinger equation is

$$i\hbar \frac{\partial \cdot \psi(q,t)}{\partial t} = -\frac{\hbar^2 \nabla^2}{2m} \psi((q,t) \tag{1.4}$$

According to the special relativity the total energy E and momenta (p_x, p_y, p_z) transform as components of a contravariant four vector

$$p^\mu = (p^0, p^1, p^2, p^3) = (\frac{E}{c}, p_x, p_y, p_z) \tag{1.5}$$

Invariant length of four momentum is

$$\sum_\mu p_\mu p^\mu = \frac{E^2}{c^2} - p^2 \equiv m^2 c^2 \tag{1.6}$$

From here we conclude that the relativistic hamiltonian is

$$H = \sqrt{p^2 c^2 + m^2 c^4}$$

(1.7)

Using this relativistic hamiltonian with the momentum operator in equation (1.3) we write the relativistic form of the Schrödinger equation as

$$i\hbar \frac{\partial \psi}{\partial t} = \sqrt{-\hbar^2 c^2 \nabla^2 + m^2 c^4}\ \psi \tag{1.8}$$

We expand the righthand-side operator in this equation as

$$\sqrt{-\hbar^2 c^2 \nabla^2 + m^2 c^4} = mc^2 (1 - \frac{1}{2} \frac{\hbar^2 \nabla^2}{m^2 c^2} + \ldots)$$

We obtain an equation containing all powers of the derivative operator ∇ and this equation is a nonlocal theory which is difficult to handle.

If we take the square of H in equation (1.7) we find an equation which is the relativistic form of the Schrödinger equation

$$(i\hbar \frac{\partial}{\partial t})(i\hbar \frac{\partial \psi}{\partial t}) = (-\hbar^2 c^2 \nabla^2 + m^2 c^4)\ \psi$$

$$\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2}-\nabla^2+(\frac{mc}{\hbar})^2\right]\psi=0 \tag{1.9}$$

named Klein-Gordon equation

$H=\pm\sqrt{p^2c^2+m^2c^4}$ presents a negative energy root appearing with a minus sign which gives the negative energy solutions of antiparticles.

Now we will try to find a conserved current from the Klein-Gordon equation. First multiplying equation (1.9) from left by $\psi*$; secondly taking hermitian conjugate of this equation and then multiplying this from left-side by ψ ,finally subtracting the latter from the former and making some calculations we obtain

$$\partial^\mu\left[\psi^*\partial_\mu\psi-\psi\partial_\mu\psi^*\right]=0 \tag{1.10}$$

or, in explicit form

$$\frac{\partial}{\partial t}\left[\frac{i\hbar}{2mc^2}(\psi^*\frac{\partial\psi}{\partial t}-\psi\frac{\partial\psi^*}{\partial t})\right]+\nabla\cdot\frac{\hbar}{2im}\left[\psi^*\nabla\psi-\psi\nabla\psi^*\right]=0 \tag{1.11}$$

The terms in the first paranthesis in equation (1.11) looks like a probability density ρ, but it is not because it is not a positive definite expression . On the other hand , equation (1.9) gives negative energy solutions in physical interpretation , so it is a strong member for transition from nonrelativistic quantum theory to a relativistic quantum mechanics as the Dirac equation which we will now discuss .

1.3 The Dirac Equation

In 1928, Dirac found a relativistic equation with the form of time dependence as in the Schrödinger equation with positive definite probability density. Because of linearity of such an equation in the time-derivative it is necessary to find an equation of linear in space derivatives. This equation is assumed to be in the form of

$$i\hbar\frac{\partial\psi}{\partial t}=\frac{\hbar c}{i}\left(\alpha_1\frac{\partial\psi}{\partial x^1}+\alpha_2\frac{\partial\psi}{\partial x^2}+\alpha_3\frac{\partial\psi}{\partial x^3}\right)+\beta mc^2\psi\equiv H\psi \tag{1.12}$$

Limitations on Dirac Equation (1.12) are :

1.From the invariance of spatial rotations, the coefficients α_i cannot be simply numbers.

2. The wave function ψ is not a simple scalar.

3. The probability density $\rho=\psi^*\psi$ should be the time component of a conserved four-vector; if ρ is integrated over all space it must be an invariant.

Dirac proposed that equation (1.12) is a matrix equation. And wave functions ψ must be in the manner of spin wave functions of non-relativistic quantum mechanics. That is

$$\psi = \begin{pmatrix} \psi_1 \\ \cdot \\ \cdot \\ \cdot \\ \psi_N \end{pmatrix}$$

where α_i, β in equation (1.12) are $N\times N$ matrices. So the N-coupled first order equations corresponding to equation are:

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{\hbar c}{i}\sum_{j=1}^{N}(\alpha_J\frac{\partial\psi}{\partial x^J} + \beta mc^2)\psi = \sum_{j=1}^{N} H\,\psi_J \tag{1.13}$$

Properties of N-coupled first order equation (1.13) are:

1. It must give the correct energy-momentum relation for a free particle :

$E'^2 - p'^2c^2 = E^2 - p^2c^2$

2.It must allow a continuity equation and a probability interpretation for the wave functions ψ

3. It must be invariant under Lorentz transformations

Each component of ψ must satisfy the Klein-Gordon equation because of the correct energy-momentum relation of Dirac equation. So we write the Dirac equation in the form of the Klein-Gordon equation :

$$i\hbar\frac{\partial}{\partial t}(i\hbar\frac{\partial\psi}{\partial t}) = \left[\frac{\hbar c}{i}\sum_{j=1}^{3}\alpha_j\frac{\partial}{\partial x^j} + \beta mc^2\right]\left[\frac{\hbar c}{i}\sum_{i=1}^{3}\alpha_i\frac{\partial}{\partial x^i} + \beta mc^2\right]\psi$$

After rearrangement we get an equation of the form

$$-\hbar^2\frac{\partial^2\psi}{\partial t^2}=-\hbar^2c^2\sum_{i,j=1}^{3}\left(\frac{\alpha_i\alpha_j+\alpha_j\alpha_i}{2}\frac{\partial^2\psi}{\partial x^i\partial x^j}\right)+\frac{\hbar mc^3}{i}\sum_{i=1}^{3}\left(\alpha_i\beta+\beta\alpha_i\right)\frac{\partial\psi}{\partial x^i}+\beta^2m^2c^4\psi \tag{1.14}$$

We take $\left(\alpha_i\alpha_j+\alpha_j\alpha_i\right)/2$ instead of $\alpha_i\alpha_j$ because we do not know that they are commutative or anticommutative .

If we compare equation (1.14) with equation (1.9) we can write that

$$\begin{aligned}&\alpha_i\alpha_j+\alpha_j\alpha_i=2\delta_{ij}\\&\alpha_i\beta+\beta\alpha_i=0\\&\alpha_i^{\ 2}=\beta^2=1\end{aligned} \tag{1.15}$$

According to nonrelativistic quantum mechanics postulates, hamiltonian seen in equation (1.13) must be a hermitian operator . So α_i, and β must be hermitian matrices. α_i, and β have the matrix form of

$$\alpha_i=\begin{pmatrix}0&\sigma_i\\\sigma_i&0\end{pmatrix},\ \beta=\begin{pmatrix}1&0\\0&-1\end{pmatrix} \tag{1.16}$$

Here σ_i are the Pauli 2×2 matrices , 1 is a 2×2 unit matrix . They are

$$\sigma_x=\begin{pmatrix}0&1\\1&0\end{pmatrix},\ \sigma_y=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\ \sigma_z=\begin{pmatrix}1&0\\0&-1\end{pmatrix},\ 1=\begin{pmatrix}1&0\\0&1\end{pmatrix} \tag{1.17}$$

To find out a current conservation equation from equation (1.13) we take the hermitian conjugate wave functions $\psi^*=(\psi^*{}_1\ldots\psi^*{}_4)$, and then we multiply equation (1.13) by ψ^+ from left and find

$$i\hbar\psi^+\frac{\partial\psi}{\partial t}=\frac{\hbar c}{i}\sum_{j=1}^{3}\psi^+\alpha_j\frac{\partial\psi}{\partial x^j}+mc^2\psi^+\beta\psi \qquad \mathrm{I}$$

Now we take hermitian conjugate of equation (1.13) and then multiplying it by ψ from right-side we obtain

$$-i\hbar\frac{\partial\psi^+}{\partial t}\psi=-\frac{\hbar c}{i}\sum_{j=1}^{3}\frac{\partial\psi^+}{\partial x^j}\alpha^+{}_j\psi+mc^2\psi^+\beta\psi \qquad \mathrm{II}$$

where $\alpha_i^+=\alpha$, $\beta^+=\beta$. Subtracting equation II from equation I we get

$$i\hbar\left[\psi^{+}\frac{\partial\psi}{\partial t}+\frac{\partial\psi^{+}}{\partial t}\psi\right]=\frac{\hbar c}{i}\sum_{j=1}^{3}\left[\psi^{+}\alpha_{j}\frac{\partial\psi}{\partial x^{j}}+\frac{\partial\psi^{+}}{\partial x^{j}}\alpha_{j}\psi\right]$$

The terms in brackets on lefthand- side is the probability density , ρ , the terms in bracket on the righthand-side is current density , $j^{k}=\Psi^{+}c\alpha^{k}\Psi$. By putting these in their places in the last equation we obtain the continuity equation

$$\frac{\partial\rho}{\partial t}+\nabla.j=0 \qquad (1.18)$$

Integrating equation (1.18) over all space we write

$$\frac{\partial}{\partial t}\int\rho d^{3}x+\sum_{j=1}^{3}\frac{\partial}{\partial x^{j}}\int\psi^{+}c\alpha^{j}\psi d^{3}x=0$$

We note that in the second term integration gives zero . Then the first term is also zero . As we see ρ is a positive definite probability density .

The density and current in equation (1.18) must be invariant under Lorentz transformation . Therefore, the probability density ρ and current j form a four-vector under this transformation .

1.4 Nonrelativistic Approach to Dirac Equation

We consider a free electron at rest and try to solve the Dirac equation for this electron. In this case , the Dirac equation is

$$i\hbar\frac{\partial\psi}{\partial t}=\beta mc^{2}\psi \qquad (1.19)$$

By using matrix form of β and ψ we write equation (1.19) in the form

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{pmatrix}=mc^{2}\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{pmatrix} \qquad (1.20)$$

From here we find out that the components of wave functions have to be

$$\psi_1 = e^{-imc^2t/\hbar}\begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \psi_2 = e^{-imc^2t/\hbar}\begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \psi_3 = e^{imc^2t/\hbar}\begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \psi_4 = e^{imc^2t/\hbar}\begin{pmatrix}0\\0\\0\\1\end{pmatrix} \quad (1.21)$$

Where ψ_1 and ψ_2 give positive energy solutions , ψ_3 and ψ_4 give negative energy solutions .

We are trying to find out an equation of Pauli spin theory by the reduction of the Dirac equation . To do this we describe a four-potential A^{μ} and a four-momentum $p^{\mu} - (e/c)A^{\mu}$ of gauge invariant form replacing p^{μ} to introduce the interaction of point charge with applied external electromagnetic field . Now Dirac equation takes the form

$$i\hbar\frac{\partial\psi}{\partial t} = \left[c\vec{\alpha}.\left(\vec{p} - \frac{e}{c}\vec{A}\right) + \beta mc^2 + e\Phi\right]\psi \quad (1.22)$$

This last equation express the interaction of a point particle with an applied electromagnetic field . The classical partner of the hamiltonian in this equation is $H = H_0 + H'$ where $H' = -e\vec{\alpha}.\vec{A} + e\Phi$. From here we note that classical hamiltonian is $H'_{classical} = -\frac{e}{c}\vec{v}.\vec{A} + e\Phi$

For the wave function in Dirac equation we introduce a wave function of two-component column matrices as

$$\psi = e^{\frac{-imc^2t}{\hbar}}\begin{pmatrix}\varphi\\ \chi\end{pmatrix}$$

Putting this two-component column matrices instead of ψ in equation (1.22) after some calculations we obtain

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\varphi\\ \chi\end{pmatrix} = c\vec{\sigma}.\vec{\pi}\begin{pmatrix}\varphi\\ \chi\end{pmatrix} - 2mc^2\begin{pmatrix}0\\ \chi\end{pmatrix} + e\varphi\begin{pmatrix}\varphi\\ \chi\end{pmatrix} \quad (1.23)$$

where $\pi = p-(e/c)A$. If we take small component χ in terms of large one φ as

$$\chi = \frac{\vec{\sigma}.\vec{\pi}}{2mc}\varphi \tag{1.24}$$

and put this instead of χ seen in equation (1.23) and use the identity

$$\vec{\sigma}.a\vec{\sigma}.b = \vec{a}.\vec{b} + i\vec{\sigma}.\vec{a}\times\vec{b} \tag{1.25}$$

to calculate $\vec{\sigma}.\vec{\pi}\vec{\sigma}.\vec{\pi} = \pi^2 + i\vec{\sigma}.\vec{\pi}\times\vec{\pi}$ and put its value in the equation, we find out two-linear equations . One of them is a two-component spinor equation ; that is

$$i\hbar\frac{\partial\psi}{\partial t} = \left[\frac{(\vec{p}-\frac{e}{c}\vec{A})^2}{2m} - \frac{e\hbar}{2mc}\vec{\sigma}.\vec{B} + e\varphi\right]\psi \tag{1.26}$$

This equation is the Pauli equation .

Neglecting higher order terms in equation (1.26) and using $\vec{r}\times\vec{p} = \vec{L}$, $\vec{A} = \frac{1}{2}\vec{r}\times\vec{B}$ in expansion of π^2; omitting field interaction which has small effect, and putting $\vec{S} = \frac{1}{2}\hbar\vec{\sigma}$ for the electron spin momentum, we reduce the Pauli equation in the form

$$i\hbar\frac{\partial\varphi}{\partial t} = \left[\frac{p^2}{2m} - \frac{e}{2mc}(2\vec{S}+\vec{L}).\vec{B}\right]\varphi \tag{1.27}$$

This last equation is the corresponding nonrelativistic equation to Dirac equation which gives correct reults .

CHAPTER 2

THE FOLDY-WOUTHUYSEN TRANSFORMATIONS

2.1 Foldy-Wouthuysen Transformation of Free Particle

We consider the hamiltonian of the Dirac equation for the free particle given by

$$H = \beta mc^2 + c\vec{\alpha}.\vec{p}$$

$$\vec{p} \rightarrow -i\hbar\vec{\nabla}$$

In our calculations we take $c = \hbar = 1$, then

$$H = \beta m + \vec{\alpha}.\vec{p}, \ \vec{p} \rightarrow -i\vec{\nabla} \qquad (2.1)$$

The matrices used in this hamiltonian are Dirac matrices .

Pauli matrices have the properties

$$[\sigma_x , \sigma_y] = 2i\sigma_z \qquad (2.2)$$

$$\sigma^2_x = \sigma_y^2 = \sigma^2_z = 1$$

In the hamiltonian written in equation (2.1), α matrices couple the small and large components of the wave function . Therefore, we will try to make a transformation to remove all odd operators represented by α from the Dirac equation . The remaining operators seen in the hamiltonian obtained under such a transformation must be even operators which don't couple small and large components of the wave function . We start to build up this transformation by the transformed wave function ψ'.ψ' is related to original wave function ψ by

$$\psi' = e^{iS}\psi \qquad (2.3)$$

Where $S=S^+$, that is, S is hermitian , and not explicitly time-dependent . Using Dirac equation for the transformed wave function ψ' we write

$$i\frac{\partial\psi}{\partial t} = H'\psi' \quad (2.4)$$

Putting equation (2.3) in equation (2.4) we obtain the transformed hamiltonian as

$$H' = e^{iS}He^{-iS} \quad (2.5)$$

where H is given by equation (2.1).

Our purpose is to obtain the hamiltonian H' in a form of even operators such as β and free of odd operators such as α.

We write e^{iS} in terms of odd operators as

$e^{iS} = e^{\beta\vec{\alpha}.\vec{p}\theta(\vec{p})}$ Where $\beta\alpha_i = \gamma_i$ are the Dirac matrices . The anticommutation relation between γ's is

$$\gamma_i\gamma_j + \gamma_j\gamma_i = 2g_{ij},$$

where

$$g_{ij} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \qquad i,j = 0,1,2,3 \qquad (2.6)$$

Before expanding e^{iS} in power series we write the unit vector for momentum-space as $\hat{n} = \frac{\vec{p}}{|\vec{p}|}$

then $\beta\vec{\alpha}.\vec{p}\theta(\vec{p}) = \sum_{i=1}^{3}\gamma_i n_i|\vec{p}|\theta(\vec{p}) = \gamma_i n_i|\vec{p}|\theta(\vec{p})$

Now we are ready to expand it . In expansion we use A for $\gamma_i n_i \gamma_j n_j$

$$e^{iS} = e^{\gamma_i n_i|\vec{p}|\theta(\vec{p})} = \sum_{k=0}^{\infty}(\gamma_i n_i)^k \frac{(|\vec{p}|\theta(\vec{p}))^k}{k!} = 1 + \gamma_i n_i|\vec{p}|\theta(\vec{p}) + \gamma_i n_i \gamma_j n_j \frac{(|\vec{p}|\theta(\vec{p}))^2}{2!} + \ldots$$

We calculate A by using equation (2.6) , i.e.,

$$A = \frac{1}{2}\left(\gamma_i\gamma_j n_i n_j + \gamma_j\gamma_i n_i n_j\right) = g_{ij}; i,j = 1,2,3, g_{ij} = -\delta_{ij},\ n_i n_j = 1$$

Then $A^2 = 1$, $A^3 = -1$,and so on . Putting values of A in expansion we obtain it

$$e^{iS}=1+\frac{\beta\vec{\alpha}.\vec{p}}{|\vec{p}|}|\vec{p}|\theta(\vec{p})-\frac{(|\vec{p}|\theta(\vec{p}))^2}{2!}-\frac{\beta\vec{\alpha}.\vec{p}}{|\vec{p}|}\frac{(|\vec{p}|\theta(\vec{p}))^3}{3!}+...$$

It can be written in the short form as

$$e^{iS}=\cos(|\vec{p}|\theta(\vec{p}))-\frac{\beta\vec{\alpha}.\vec{p}}{|\vec{p}|}\sin(|\vec{p}|\theta(\vec{p})) \qquad (2.7)$$

In the same way we write

$$e^{-iS}=\cos(|\vec{p}|\theta(\vec{p}))-\frac{\beta\vec{\alpha}.\vec{p}}{|\vec{p}|}\sin(|\vec{p}|\theta(\vec{p})) \qquad (2.8)$$

By putting equations (2.1), (2.7), and (2.8) in equation (2.5) we make the following calculation:

$$H'=[\cos(|\vec{p}|\theta)+\frac{\beta\vec{\alpha}.\vec{p}}{|\vec{p}|}\sin(|\vec{p}|\theta)][\beta m+\vec{\alpha}.\vec{p}][\cos(|\vec{p}|\theta)-\sin(|\vec{p}|\theta)]$$

We make some calculations to write H' in explicit terms by using anticommutation relation between β *and* α, i.e.,$\{\beta,\alpha\}=0$, and $\beta^2=1$. We rewrite the above equation after some rearrangement in its terms as

$$H'=\beta[m\cos(2|\vec{p}|\theta)+|\vec{p}|\sin(2|\vec{p}|\theta)]+\vec{\alpha}.\vec{p}[\cos(2|p|\theta)-\frac{m}{|\vec{p}|}\sin(2|p|\theta)] \qquad (2.9.1)$$

To eliminate the odd operators in the last equation we equalize the terms in the second bracket to zero .That is

$$\cos(2|\vec{p}|\theta)-\frac{m}{|\vec{p}|}\sin(2|\vec{p}|\theta)=0$$

from here we obtain

$$\tan(2|\vec{p}|\theta)=\frac{m}{|\vec{p}|}$$

By using the trigonometric relation $\cos^2\theta+\sin^2\theta=1$ with this last equation we reduce equation (2.9.1) to

$$H'=\beta\sqrt{m^2+p^2} \qquad (2.9.2)$$

In the last equation hamiltonian H' is free of odd operators . Moreover , it is in the form of relativistic free particle hamiltonian $H=\sqrt{m^2+p^2}$. The difference is that H' has negative-energy solutions as well as the positive energy-solutions which the relativistic hamiltonian possesses .

2.2. The General Foldy-Wouthuysen Transformation

Now we are considering an electron with a given electromagnetic field . In this case the hamiltonian is

$$H = c\vec{\alpha}.\vec{p} + \beta mc^2 + e\varphi$$

Setting $c=\hbar=1$, and $O=\vec{\alpha}.\vec{\pi}$ to denote the odd operators of the hamiltonian , and $E = e\varphi$ to denote the even part of the hamiltonian we write

$$H = \beta m + E + O \qquad (2.10)$$

Odd operators anticommute with β ,i.e., $\{\beta, O\} = 0$, and even operators commute with it , i.e., $[\beta, E] = 0$

The fields under consideration are time-dependent hence the hamiltonian H itself also is time-dependent . Again we make a transformation of the form e^{iS} . In this case, S is time-dependent. To construct an S transformation that removes all odd operators in the new hamiltonian is not like what we did in the free particle transformation . Therefore , we take S in the order of $\frac{1}{m}$, and keeping terms up to the order $\frac{1}{m^2}$ and $\frac{1}{m^3}$ in the transformed hamiltonian we overcome this problem . Now with S time-dependent, we write transformed wave function $\psi' = e^{iS}\psi$ as the starting point of construction of the general Foldy-Wouthuysen transformation . Again we use

$$i\frac{\partial \psi'}{\partial t} = H'\psi' \qquad \text{with } \psi' = e^{iS}\psi$$

Putting $e^{iS}\ \psi$ in its place we continue as follows:

$$i\frac{\partial}{\partial t}(e^{iS}\psi) = H'e^{iS}\psi$$

$$(i\frac{\partial e^{iS}}{\partial t})\psi + e^{iS}(i\frac{\partial \psi}{\partial t}) = H'e^{iS}\psi$$

where $i\frac{\partial \psi}{\partial t} = H\psi$

Rewritting the last equation we obtain

$$H'e^{iS} = (i\frac{\partial}{\partial t}e^{iS}) + e^{iS}H$$

Multiplying this equation from right by e^{-iS} we obtain H' as

$$H' = (i\frac{\partial}{\partial t}e^{iS})e^{-iS} + e^{iS}He^{-iS} \tag{2.11}$$

Now we write e^{iS} and e^{-iS} in their expansion form

$$e^{iS} = \sum_{n=0}^{\infty}\frac{i^n}{n!}S^n = 1 + iS + \frac{i^2}{2!}S^2 + \ldots$$

$$e^{-iS} = \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}S^n = 1 - iS + \frac{i^2}{2!}S^2 + \ldots$$

First we put these values in the second term of equation (2.11). That is

$$e^{iS}He^{-iS} = H + i[S,H] + \frac{i^2}{2!}[S,[S,H]] + \ldots \tag{2.12}$$

Here we used $e^{A}Be^{-A} = \sum_{n=0}^{\infty}\frac{1}{n!}[A,[A,[\ldots[A,B]\ldots]]]$

And then putting values of the expansion in the first term of equation (2.11) after some arrangement of terms we write

$$(i\frac{\partial}{\partial t}e^{iS})e^{-iS} = -\frac{\partial S}{\partial t} - \frac{i}{2}[S,\frac{\partial S}{\partial t}] + \ldots \tag{2.13}$$

When equations (2.12), and (2.13) are written in their places in equation (2.11) the transformed hamiltonian H' becomes

$$H' = H + i[S,H] + \frac{i^2}{2!}[S,[S,H]] + \ldots - \frac{\partial S}{\partial t} - \frac{i}{2!}[S,\frac{\partial S}{\partial t}] - \frac{i^2}{3!}[S,[S,\frac{\partial S}{\partial t}]] - \ldots$$

We choose $S=-\frac{i\beta O}{2m}$. Using the hamiltonian of equation (2.10) and making some calculations to the mentioned orders we rewrite the transformed hamiltonian H' as

$$H'=\beta m+E+\frac{\beta O^2}{2m}-\frac{1}{8m^2}([O,[O,E]]+i[O,\dot{O}])-\frac{\beta O^4}{8m^3}+...+\frac{\beta}{2m}[O,E]+\frac{i\beta}{2m}O-\frac{O^3}{3m^2}+...$$

Now in the transformed hamiltonian we have odd terms and even terms . We denote them by O' and E' . They are

$$O'=\frac{\beta}{2m}[O,E]+\frac{i\beta}{2m}O-\frac{O^3}{3m^2} \tag{2.14}$$

$$E'=E+\frac{\beta O^2}{2m}-\frac{1}{8m^2}([O,[O,E]]+i[O,\dot{O}])-\frac{\beta O^4}{8m^3} \tag{2.15}$$

In terms of E' and O' the new hamiltonian is

$$H'=\beta m+O'+E' \tag{2.16}$$

We conclude that the coefficients of the odd terms begin with $\frac{1}{m}$. Therefore ,we are going to make a second transformation in the same manner with $S'=-\frac{i\beta O'}{2m}$.

$$H''=e^{iS'}H'e^{-iS'}+\left[i\frac{\partial}{\partial t}e^{iS''}\right]e^{-iS'} \tag{2.17}$$

$$e^{iS'}=\left[1+iS'-\frac{1}{2}S'^2-\frac{1}{3}S'^3+...\right]$$

$$e^{-iS'}=\left[1-iS'-\frac{1}{2}S'^2-...\right]$$

The first term on the right side of equation (2.17) is

$$e^{iS'}H'e^{-iS'}=H'+i[S',H'] \tag{2.18}$$

The second term is

$$\left[i\frac{\partial}{\partial t}e^{iS'}\right]e^{-iS'}=-\frac{\partial S'}{\partial t}-\frac{i}{2}\left[S',\frac{\partial S'}{\partial t}\right]+... \tag{2.19}$$

Putting eqns. (2.18) and (2.19) in eqn. (2.17) we obtain the second transformed hamiltonian as

$$H'' = H' + i[S', H'] - \frac{\partial S'}{\partial t} + \ldots$$

Using values of S' and H' we find

$$i[S', H'] = -O' + \frac{\beta}{2m}[O', E'] + \frac{\beta O'^2}{m}$$

where $-\frac{\partial S'}{\partial t} = \frac{i\beta \dot{O}'}{2m}$

Then transformed H'' takes the form

$$H'' = \beta m + E' + \frac{\beta}{2m}[O', E'] + \frac{i\beta \dot{O}'}{2m}$$

$$H'' = \beta m + E' + O''$$

where we introduce

$$O'' = \frac{\beta}{2m}[O', E'] + \frac{i\beta \dot{O}'}{2m}$$

Comparing the odd operator O'' with the order of $1/m$ we see that O'' is in the order of $1/m^2$. To get an order of $1/m^3$ for the transformed hamiltonian we make a third transformatian with $S'' = -\frac{i\beta O''}{2m}$. That is

$$H''' = e^{iS''} H'' e^{-iS''} + \left[i \frac{\partial}{\partial t} e^{iS''} \right] e^{-iS''}$$

$$H''' = H'' + i[S'', H''] + \ldots$$

$$i[S'', H''] = -O'' + \frac{\beta}{2m}[O'', E'] + \frac{\beta}{m} O''^2$$

Then the transformed hamiltonian is

$$H''' = \beta m + E' + \frac{\beta}{2m}[O'', E'] + \frac{\beta}{2m} O''^2 + \ldots$$

Neglecting the terms greater than order of $1/m^3$ we write the transformed hamiltonian as

$$H''' = \beta m + E' \tag{2.20}$$

Putting equation (2.14) in equation (2.20) the explicit transformed hamiltonian is

$$H''' = (\beta m + \frac{\beta O^2}{2m} - \frac{\beta O^4}{8m^3}) + E - \frac{1}{8m^2}[O,[O,E]] - \frac{i}{8m^2}\left[O,\dot{O}\right] \quad (2.21)$$

After calculation of each term in transformed hamiltonian H''' we get explicitly

$$\frac{O^2}{2m} = \frac{(\vec{\alpha}.\vec{\pi})^2}{2m} = \frac{\left[\vec{\alpha}.(\vec{p}-e\vec{A})\right]^2}{2m} = \frac{(\vec{p}-e\vec{A})^2}{2m} - \frac{e}{2m}\vec{\sigma}.\vec{B}$$

$$\frac{1}{8m^2}\left[O,([O,E]+i\dot{O})\right] = -\frac{e}{8m^2}\vec{\nabla}.\vec{E} - i\frac{e}{8m^2}\vec{\sigma}.\vec{\nabla}\times\vec{E} - \frac{e}{4m^2}\vec{\sigma}.\vec{E}\times\vec{p}$$

where E used on the lefthand- side denotes even operator and that used on the right-hand side the electiric field. And we use $\vec{p} = -i\vec{\nabla}, \vec{B} = \vec{\nabla}\times\vec{A}$, and $\vec{E} = -\vec{\nabla}\Phi - \dot{\vec{A}}$ in our calculations . Substituting each explicit term in its place we get the transformed hamiltonian as

$$H''' = \beta\left[m + \frac{(\vec{p}-e\vec{A})^2}{2m} - \frac{p^4}{8m^3}\right] + (e\Phi - \frac{e}{2m}\beta\vec{\sigma}.\vec{B}) - \frac{ie}{8m^2}\sigma.\vec{\nabla}\times\vec{E} - \frac{e}{4m^2}\vec{\sigma}.\vec{E}\times\vec{p} - \frac{e}{8m^2}\vec{\nabla}.\vec{E} \quad (2.22)$$

The first term is the expansion of $\sqrt{(\vec{p}-e\vec{A})^2+m^2}$ to the effective order of interaction and this term corresponds to the relativistic mass increase .

The second term is the electrostatic energy and magnetic dipole energy respectively .

The third and fourth terms are the spin-orbit interaction energy terms. In a spherically symmetric potential electric field in terms of the static potential is

$$\vec{E} = -\frac{\vec{r}}{|\vec{r}|}\frac{\partial V}{\partial r} \quad (2.23)$$

For this case, $\vec{\nabla}\times\vec{E} = 0$. Now the spin-orbit interaction energy terms take the form

$$H_{spin\text{-}orbit} = -\frac{e}{4m^2 r}\frac{\partial V}{\partial r}\vec{\sigma}.\vec{r}\times\vec{p} = \frac{e}{4m^2 r}\frac{\partial V}{\partial r}\vec{\sigma}.\vec{L} \qquad (2.24)$$

Where $\vec{L} = \vec{r}\times\vec{p}$ is the orbital angular momentum.

Clasically an electron moving in an electric field with velocity $\vec{v}$ sees an apparent magnetic field given by $\vec{B} = -\vec{v}\times\vec{E}$. The interaction energy in this case is

$$U = -\frac{e}{2m}\vec{\sigma}.\vec{B} = -\frac{e}{2m^2}\vec{\sigma}.\vec{p}\times\vec{E} \qquad (2.25)$$

If we use the electric field given by equation (2.23) the interaction energy in classical consideration is

$$U = \frac{e}{2m^2 r}\frac{\partial V}{\partial r}\vec{\sigma}.\vec{L} \qquad (2.26)$$

By comparing the energy found in equation (2.26) to that of equation (2.24) we note that the relativistic spin-orbit interaction is in the form of classical interaction and is reduced by the factor of 2.

The last term in equation (2.22) is the Darwin term. Darwin term is connected to Zitterbewegung which indicates an oscillatory motion with a frequency of $2H/\hbar$. Since the electron coordinate fluctuates over a distance of δr we need a correction of potential in average value as

$$<\delta V> = <V(\vec{r}+\vec{\delta r})> - <V(\vec{r})>$$

Using $<V(\vec{r}+\delta\vec{r})> = <V(\vec{r})> + <\delta\vec{r}.\vec{\nabla}V> + \frac{1}{2}\sum_{i,j}\delta r_i\delta r_j\frac{\partial^2 V}{\partial r_i\partial r_j}$ we find out

$$<\delta V> = <\frac{1}{2}\sum_{i,j}\delta r_i\delta r_j\frac{\partial^2 V}{\partial r_i\partial r_j}>$$

$$<\delta V> \cong \frac{1}{6m^2}\nabla^2 V \qquad (2.27)$$

Where we use $\delta r \approx \frac{1}{m}$

After the discussion of the physical meaning of terms seen in the transformed hamiltonian we are going to reduce it for a wave function of two two-component wave functions. We introduce the wave function as

$$\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \tag{2.28}$$

Where φ corresponds to the large components of the wave functions and χ to that of small components .

Acting the hamiltonian of equation (2.22) on the wave function ψ we make the following

$$i\frac{\partial}{\partial t}\begin{bmatrix} \varphi \\ \chi \end{bmatrix} = \left\{ \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} (m + \frac{(\vec{p} - e\vec{A})^2}{2m} - \frac{p^4}{8m^3} - \frac{e}{2m}\vec{\sigma}.\vec{B}) + e.\phi - \frac{ie}{8m^2}\vec{\sigma}.\vec{\nabla} \times \vec{E} \right.$$

$$\left. - \frac{e}{4m^2}\vec{\sigma}.\vec{E} \times \vec{p} - \frac{e}{8m^2}\vec{\nabla}.\vec{E} + \ldots\ldots\ldots \right\} \begin{bmatrix} \varphi \\ \chi \end{bmatrix} \tag{2.29}$$

From here we obtain two equations . The equation of the large component give the positive energy solutions of the Dirac equation , and is reduced to the Pauli-Schrödinger equation in the nonrelativistic consideration . If we drop the rest energy in this equation and keep terms $\frac{\pi^2}{2m} - \frac{e}{2m}\vec{\sigma}.\vec{B} + e\phi$ of the hamiltonian it reduces to the Pauli-Schrödiger equation .

Equation of the small components give the negative energy solutions of the Dirac equation.

CHAPTER 3

THE HYDROGEN ATOM

3.1. The Hydrogen Atom

Now we are dealing with energy levels of the electron in a central field such as in a Coulomb field. The Dirac equation for such a bound-state, i.e., E<0 is

$$\mathrm{H}\psi = [\vec{\alpha}.\vec{p} + \beta m + V(r)]\psi = E\psi \qquad (3.1)$$

where $V(r) = -\dfrac{Z\alpha}{r}$, and $\alpha = \dfrac{e^2}{\hbar c}$

We note that the angular momentum of a particle in a central field is conserved. Total angular momentum is the sum of orbital angular momentum and spin momentum, i.e.,

$$\vec{J} = \vec{L} + \vec{S} \text{ with } \vec{S} = \frac{1}{2}\vec{\sigma} \qquad (3.2)$$

Since the total angular momentum is conserved it must commute with the hamiltonian given in equation (3.1). We are going to check this fact;

$$[H, \vec{J}] = \left[\vec{\alpha}.\vec{p} + \beta m + V(r), \vec{L} + \frac{1}{2}\vec{\sigma}\right]$$

$$[\vec{\alpha}.\vec{p} + \beta m + V(r), \vec{L}] + \frac{1}{2}[\vec{\alpha}.\vec{p} + \beta m + V(r), \vec{\sigma}]$$

where σ is a 4×4 matrix in terms of Pauli matrices. First of all we choose $L_1 = x_2 p_3 - x_3 p_2$

$$[H, L_1] = [\beta m + \alpha_j P_j + V(r), x_2 p_3 - x_3 p_2]$$

$$[H, L_1] = -i\alpha_j (\delta_{2j} p_3 - \delta_{3j} p_2) = -i\alpha_2 p_3 + i\alpha_3 p_2$$

We generalize this result as

$$[H, L] = i\vec{\alpha} \times \vec{p} \tag{3.3}$$

From here we conclude that $\vec{L}$ is not a constant of motion.

Dirac Matrices

Dirac matrices are; $\gamma^k = \beta\alpha_k = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_k \\ -\sigma_k & 0 \end{pmatrix}$

$$\gamma^1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \qquad \gamma^2 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix} \tag{3.4}$$

$$\gamma^3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \qquad \gamma^5 = \gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

Now we turn to the consistancy of angular momentum. This time we search for consistancy of $\vec{S} = \frac{1}{2}\vec{\sigma}$ where $\vec{\sigma}$ is a 4×4 matrix. We must use

$$-\gamma_5\vec{\sigma} = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}\begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix} = \begin{pmatrix} 0 & \sigma \\ 0 & 0 \end{pmatrix} = \vec{\alpha} = -\vec{\sigma}\gamma_5$$

We first take σ_x and setting $\vec{\alpha} = -\gamma_5 \sigma$ in $[H, S]$.

Then we get

$$[\vec{\alpha}.\vec{p} + \beta m + V(r), \sigma_x] = [\vec{\alpha}.\vec{p}, \sigma_x] = [-\gamma_5 \sigma_j p_j, \sigma_x].$$

Using $[\sigma_x, \sigma_y] = 2i\sigma_z$, and $\sigma_x{}^2 = \sigma_y{}^2 = \sigma_z{}^2 = 1$ and we obtain

then

$$[\vec{\alpha}.\vec{p}, \sigma_x] = \begin{bmatrix} 0 & 2i\sigma_z \\ 2i\sigma_z & 0 \end{bmatrix} p_y + \begin{bmatrix} 0 & -2i\sigma_y \\ -2i\sigma_y & 0 \end{bmatrix} p_z$$

then

$$[\vec{\alpha}.\vec{p}, \sigma_x] = 2i\alpha_z p_y - 2i\alpha_y p_z$$

We generalize this result as

$$[\vec{\alpha}.\vec{p}, \vec{\sigma}] = -2i\vec{\alpha} \times \vec{p} \qquad (3.5)$$

We conclude that $\vec{S} = \frac{1}{2}\vec{\sigma}$ is not a constant of motion. We now combine equation (3.3) and equation (3.5) and obtain

$$\begin{aligned}[H, \vec{J}] &= \left[\vec{\alpha}.\vec{p} + \beta m + V(r), \vec{L} + \frac{1}{2}\vec{\sigma}\right] \\ &= -i\vec{\alpha} \times \vec{p} + i\vec{\alpha} \times \vec{p} = 0 \end{aligned} \qquad (3.6)$$

We have to build up a wave function which is simultaneous eigenfunction of H, J^2, and, J_z. It must be a wave function of two-component spinors, i.e.,

$$\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \qquad (3.7)$$

φ and χ are two-component spinors in the form of two-component Pauli theory. They are in two forms.

For $J = l + \frac{1}{2}$

$$\varphi_{J,m}^{(+)} = \begin{pmatrix} \sqrt{\dfrac{l+m+\frac{1}{2}}{2l+1}}\varphi_l^{m-\frac{1}{2}} \\ \sqrt{\dfrac{l-m+\frac{1}{2}}{2l+1}}\varphi_l^{m+\frac{1}{2}} \end{pmatrix} \tag{3.8}$$

For $J = l - \frac{1}{2}$

$$\varphi_{J,m}^{(-)} = \begin{pmatrix} \sqrt{\dfrac{l-m+\frac{1}{2}}{2l+1}}\varphi_l^{m-\frac{1}{2}} \\ -\sqrt{\dfrac{l+m+\frac{1}{2}}{2l+1}}\varphi_l^{m+\frac{1}{2}} \end{pmatrix} \tag{3.9}$$

Both of the eigenfunctions must satisfy the eigenvalues of J^2, L^2, S^2, and J_z. We write them down.

$$J^2 \varphi_{J,m}^{\pm} = J(J+1)\varphi_{J,m}^{\pm}$$

$$\vec{\sigma}.\vec{L}\varphi_{J,m}^{\pm} = \left[J(J+1) - l(l+1) - \frac{3}{4}\right]\varphi_{J,m}^{\pm} = -(1+\kappa)\varphi_{J,m}^{\pm} \tag{3.10}$$

If $J = l + \frac{1}{2}$

$$-(1+\kappa)=\left[\left(l+\frac{1}{2}\right)\left(l+\frac{3}{2}\right)-l(l+1)-\frac{3}{4}\right]$$

$$-(1+\kappa)=l \text{ or } \kappa=-(l+1) \tag{3.11}$$

If $J=l-\frac{1}{2}$

$$-(1+\kappa)=\left[\left(l-\frac{1}{2}\right)\left(l+\frac{1}{2}\right)-l(l+1)-\frac{3}{4}\right]$$

$$\kappa=l \tag{3.12}$$

$\varphi^{(+)}_{J,m}$ and $\varphi^{(-)}_{J,m}$ have opposite parities for a given J because their orbital angular momentum differ by one unit, i.e., when $J=l+\frac{1}{2}$, $\varphi^{l}_{J,m}$ is denoted by $\varphi^{(+)}_{J,m}$ and when $J=l-\frac{1}{2}$, $\varphi^{l}_{J,m}$ is denoted by $\varphi^{(-)}_{J,m}$. $\varphi^{l}_{J,m}$ has parity $(-1)^{l}$. $\varphi^{(+)}_{J,m}$ and $\varphi^{(-)}_{J,m}$ can be formed from each other by a scalar operator. This operator is $\frac{\vec{\sigma}\vec{r}}{r}$ which is a pseudoscalar. We write this fact as

$$\varphi^{(+)}_{J,m}=\frac{\vec{\sigma}\vec{r}}{r}\varphi^{(-)}_{J,m}. \tag{3.13}$$

The Dirac equation in the Coulomb field is invariant under space reflection, therefore we can write odd and even eigenstates of parity under the transformation $x'=-x$ as

$$\psi'(x')=\beta\psi^{(\pm)}_{J,m}(x)=\pm\psi^{(\pm)}_{J,m}(x) \tag{3.14}$$

We write $\psi^{l}_{J,m}$ as below

$$\psi^{l}_{J,m}=\begin{pmatrix}\dfrac{iG_{IJ}}{r} & \varphi^{l}_{J,m}\\ \dfrac{F_{IJ}}{r} & \dfrac{\vec{\sigma}.\vec{r}}{r}\varphi^{l}_{J,m}\end{pmatrix} \tag{3.15}$$

G_{IJ} and F_{IJ} denotes spatial part of the wave function.

We write hamiltonian given by equation (3.1) in explicit form as

$$H=\vec{\alpha}.\vec{p}+\beta m-\frac{Z\alpha}{r}$$

$$H=\begin{pmatrix}0 & \vec{\sigma}\\ \vec{\sigma} & 0\end{pmatrix}.\vec{p}+\begin{pmatrix}m & 0\\ 0 & -m\end{pmatrix}+\begin{pmatrix}-\dfrac{Z\alpha}{r} & 0\\ 0 & -\dfrac{Z\alpha}{r}\end{pmatrix}$$

$$H=\begin{pmatrix}m-\dfrac{Z\alpha}{r} & \vec{\sigma}.\vec{p}\\ \vec{\sigma}.\vec{p} & -m-\dfrac{Z\alpha}{r}\end{pmatrix}$$

We operate with $\vec{\sigma}.\vec{p}$ on $\dfrac{F(r)}{r}\varphi^{l}_{J,m}$ as below

$$\vec{\sigma}.\vec{p}\frac{F(r)}{r}\varphi^{l}_{J,m}=\frac{\vec{\sigma}.\vec{r}}{r^{2}}(\vec{\sigma}.\vec{r})(\vec{\sigma}.\vec{p})\frac{F(r)}{r}\varphi^{l}_{J,m}$$

$$=\frac{\vec{\sigma}.\vec{r}}{r^{2}}(\vec{r}.\vec{p}+i\vec{\sigma}.\vec{r}\times\vec{p})\frac{F(r)}{r}\varphi^{l}_{J,m}$$

$$\vec{\sigma}.\vec{p}\frac{F(r)}{r}\varphi^{l}_{J,m}=\frac{\vec{\sigma}.\vec{r}}{r^{2}}\left[-ir\frac{\partial}{\partial r}+i\vec{\sigma}.\vec{L}\right]\frac{F(r)}{r}\varphi^{l}_{J,m}$$

We find out that the eigenvalue of $\vec{\sigma}.\vec{L}$ is $-(1+\kappa)$. Then we write the above equation as

$$\vec{\sigma}.\vec{p}\frac{F(r)}{r}\varphi^{l}_{J,m}=\left[-ir\frac{d}{dr}\left(\frac{F(r)}{r}\right)-i(1+\kappa)\frac{F(r)}{r^{2}}\right]\frac{\vec{\sigma}\vec{r}}{r}\varphi^{l}_{J,m} \tag{3.16}$$

We turn to the Dirac equation again:

$$E\psi=\left[\vec{\alpha}.\vec{p}+\beta m-\frac{Z\alpha}{r}\right]\psi=H\psi$$

$$\begin{pmatrix}E & 0\\ 0 & E\end{pmatrix}\begin{pmatrix}\frac{iG_{IJ}}{r}\varphi^{l}_{J,m}\\ \frac{F_{IJ}}{r}\frac{\vec{\sigma}\vec{r}}{r}\varphi^{l}_{J,m}\end{pmatrix}=\begin{pmatrix}m-\frac{Z\alpha}{r} & \vec{\sigma}.\vec{p}\\ \vec{\sigma}.\vec{p} & -m-\frac{Z\alpha}{r}\end{pmatrix}\begin{pmatrix}\frac{iG_{IJ}}{r}\varphi^{l}_{J,m}\\ \frac{F_{IJ}}{r}\frac{\vec{\sigma}\vec{r}}{r}\varphi^{l}_{J,m}\end{pmatrix}$$

$$\begin{pmatrix}E-m+\frac{Z\alpha}{r} & -\vec{\sigma}.\vec{p}\\ -\vec{\sigma}.\vec{p} & E+m+\frac{Z\alpha}{r}\end{pmatrix}\begin{pmatrix}\frac{iG_{IJ}}{r}\varphi^{l}_{J,m}\\ \frac{F_{IJ}}{r}\frac{\vec{\sigma}\vec{r}}{r}\varphi^{l}_{J,m}\end{pmatrix}=0$$

This matrix equation is equal to the two equations below;

$$-i\frac{\vec{\sigma}.\vec{p}}{r}G_{IJ}\varphi^{l}_{J,m}+\left(E+m+\frac{Z\alpha}{r}\right)\frac{F_{IJ}}{r}\frac{\vec{\sigma}.\vec{r}}{r}\varphi^{l}_{J,m}=0$$

$$i\left(E-m+\frac{Z\alpha}{r}\right)\frac{G_{IJ}}{r}\varphi'_{J,m}-\vec{\sigma}.\vec{p}\frac{F_{IJ}}{r}\frac{\vec{\sigma}.\vec{r}}{r}\varphi'_{J,m}=0 \tag{3.17}$$

Putting equation (3.16) in equation (3.17) we proceed as follows:

$$i\left(E-m+\frac{Z\alpha}{r}\right)\frac{G_{IJ}}{r}\varphi^{l}_{J,m}+\left[\frac{d}{dr}\frac{F(r)}{r}+(1+\kappa)\frac{F(r)}{r^{2}}\right]\frac{\vec{\sigma}\vec{r}}{r}\frac{\vec{\sigma}\vec{r}}{r}\varphi^{l}_{J,m}=0$$

$$\left(E-m+\frac{Z\alpha}{r}\right)\frac{G_{IJ}}{r}=-\frac{1}{r}\frac{dF_{IJ}(r)}{dr}+\frac{F_{IJ}(r)}{r^{2}}-\frac{F_{IJ}(r)}{r^{2}}-\frac{\kappa}{r^{2}}F_{IJ}$$

$$\left(E-m+\frac{Z\alpha}{r}\right)G_{IJ}=-\frac{dF_{IJ}}{dr}-\frac{\kappa}{r}F_{IJ} \tag{3.18}$$

$$-i\frac{\vec{\sigma}.\vec{p}}{r}G_U\varphi^l_{J,m}+\left(E+m+\frac{Z\alpha}{r}\right)\frac{F_U}{r}\frac{\vec{\sigma}.\vec{r}}{r}\varphi^l_{J,m}=0$$

$$\left(E+m+\frac{Z\alpha}{r}\right)\frac{F_U}{r}\frac{\vec{\sigma}\vec{r}}{r}\varphi^l_{J,m}=i\vec{\sigma}.\vec{p}\frac{G_U}{r}\varphi^l_{J,m}$$

$$\left(E+m+\frac{Z\alpha}{r}\right)\frac{1}{r^2}F_U\vec{\sigma}\vec{r}\varphi^l_{J,m}=\frac{\vec{\sigma}\vec{r}}{r^2}[\vec{\sigma}\vec{r}\vec{\sigma}.\vec{p}]\frac{iG_U}{r}\varphi^l_{J,m}$$

$$\left(E+m+\frac{Z\alpha}{r}\right)F_U\vec{\sigma}.\vec{r}\varphi^l_{J,m}=\vec{\sigma}.\vec{r}\left[\vec{r}.\vec{p}+i\vec{\sigma}.\vec{r}\times\vec{p}\right]\frac{iG_U}{r}\varphi^l_{J,m}$$

$$\left(E+m+\frac{Z\alpha}{r}\right)F_U\vec{\sigma}.\vec{r}\varphi^l_{J,m}=\vec{\sigma}.\vec{r}\left[\vec{r}.\left(-i\frac{d}{dr}\right)+i\vec{\sigma}.\vec{L}\right]\frac{iG_U}{r}\varphi^l_{J,m}$$

Putting equation (3.10) in the latter equation we obtain

$$\left(E+m+\frac{Z\alpha}{r}\right)F_U\vec{\sigma}.\vec{r}\varphi^l_{J,m}=\left[\frac{dG_U}{dr}-\frac{G_U}{r}\right]\vec{\sigma}.\vec{r}\varphi^l_{J,m}+i(-1-\kappa)\frac{iG_U}{r}\vec{\sigma}.\vec{r}\varphi^l_{J,m}$$

$$\left(E+m+\frac{Z\alpha}{r}\right)F_U\vec{\sigma}.\vec{r}\varphi^l_{J,m}=\left[\frac{dG_U}{dr}-\frac{G_U}{r}+(1+\kappa)\frac{G_U}{r}\right]\vec{\sigma}.\vec{r}\varphi^l_{J,m}$$

$$\left(E+m+\frac{Z\alpha}{r}\right)F_U=\frac{dG_U}{dr}+\frac{\kappa}{r}G_U \qquad (3.19)$$

Now we have to solve equations (3.18), and (3.19). And on the basis of these two equations we introduce

$\alpha_1=m+E$, $\alpha_2=m-E$, $\gamma=Z\alpha$, $\rho=\sqrt{\alpha_1\alpha_2}r$

We put these values in equation (3.18) and we make following calculations;

$$d\rho = \sqrt{\alpha_1\alpha_2}dr \rightarrow dr = \frac{d\rho}{\sqrt{\alpha_1\alpha_2}}$$

$$\frac{dF_U}{dr} \mp \frac{\kappa}{r}F_U = -\left[E - m + \frac{Z\alpha}{r}\right]G_U$$

$$\sqrt{\alpha_1\alpha_2}\frac{dF_U}{d\rho} \mp \frac{\kappa\sqrt{\alpha_1\alpha_2}}{\rho}F_U = \left[\alpha_2 - \sqrt{\alpha_1\alpha_2}\frac{\gamma}{\rho}\right]G_U$$

$$\frac{dF_U}{d\rho} \mp \frac{\kappa}{\rho}F_U = \left[\sqrt{\frac{\alpha_2}{\alpha_1}} - \frac{\gamma}{\rho}\right]G_U$$

$$\frac{dF_U}{d\rho} - \frac{\kappa}{\rho}F_U = \left[\sqrt{\frac{\alpha_2}{\alpha_1}} - \frac{\gamma}{\rho}\right]G_U \tag{3.18.1}$$

As in the non-relativistic solutions of the hydrogen atom we put F_U and G_U in the power series form, i.e.,

$$F = e^{-\rho}\rho^s\sum_{m=0}^{\infty}a_m\rho^m \text{ and } G = e^{-\rho}\rho^s\sum_{m=0}^{\infty}b_m\rho^m \tag{3.20}$$

Then equation (3.18.1) can be written as

$$\left[\frac{d}{d\rho} - \frac{\kappa}{\rho}\right]e^{-\rho}\rho^s\sum_{m=0}^{\infty}a_m\rho^m - \left[\sqrt{\frac{\alpha_2}{\alpha_1}} - \frac{\gamma}{\rho}\right]e^{-\rho}\rho^s\sum_{m=0}^{\infty}b_m\rho^m = 0$$

$$e^{-\rho}\rho^{s}\sum_{m=0}^{\infty}a_m\rho^m + se^{-\rho}\rho^{s-1}\sum_{m=0}^{\infty}a_m\rho^m + e^{-\rho}\rho^{s}\sum_{m=0}^{\infty}ma_m\rho^{m-1} - \kappa e^{-\rho}\rho^{s-1}\sum_{m=0}^{\infty}a_m\rho^m$$

$$-\sqrt{\frac{\alpha_2}{\alpha_1}}e^{-\rho}\rho^{s}\sum_{m=0}^{\infty}b_m\rho^m + \gamma e^{-\rho}\rho^{s-1}\sum_{m=0}^{\infty}b_m\rho^m = 0$$

$$-\sum_{m=0}^{\infty}\left(a_m + \sqrt{\frac{\alpha_2}{\alpha_1}}b_m\right)\rho^{m+s} + \sum_{m=0}^{\infty}\left[sa_m + ma_m - \kappa a_m + \gamma b_m\right]\rho^{m+s-1} = 0$$

To write the second part to the power $m+1$ we introduce a new index $n = m-1$

$$-\sum_{m=0}^{\infty}\left(a_m + \sqrt{\frac{\alpha_2}{\alpha_1}}b_m\right)\rho^{m+s} + \sum_{m=-1}^{\infty}\left[sa_{m+1} + (m+1)a_{m+1} - \kappa a_{m+1} + \gamma b_{m+1}\right]\rho^{m+s} = 0$$

$$(sa_0 - \kappa a_0 + \gamma b_0)\rho^{s-1}$$

$$+\sum_{m=0}^{\infty}\left(sa_{m+1} + (m+1)a_{m+1} - \kappa a_{m+1} + \gamma b_{m+1} - a_m - \sqrt{\frac{\alpha_2}{\alpha_1}}b_m\right)\rho^{m+s} = 0$$

The coefficients of same power of ρ must be equal to zero. So we write

$$(s-\kappa)a_0 + \gamma b_0 = 0 \qquad (3.21)$$

$$(s+m+1-\kappa)a_{m+1} + \gamma b_{m+1} - a_m - \sqrt{\frac{\alpha_2}{\alpha_1}}b_m = 0, \quad m \geq 0$$

Here we introduce a new index $q = m+1$,

$$(s+q-\kappa)a_o+\gamma b_q=a_{q-1}+\sqrt{\frac{\alpha_2}{\alpha_1}}b_{q-1},\quad q\geq 1 \qquad (3.22)$$

In the same way we solve equation (3.19)

$$\frac{dG_U}{dr}+\frac{\kappa}{r}G_U-\left[m+E+\frac{Z\alpha}{r}\right]F_U=0$$

$$\sqrt{\alpha_1\alpha_2}\frac{dG_U}{d\rho}+\sqrt{\alpha_1\alpha_2}\frac{\kappa}{\rho}G_U-\left[\alpha_1+\frac{\gamma}{\rho}\sqrt{\alpha_1\alpha_2}\right]F_U=0$$

$$\frac{dG_U}{d\rho}+\frac{\kappa}{\rho}G_U-\left[\sqrt{\frac{\alpha_1}{\alpha_2}}+\frac{\gamma}{\rho}\right]F_U=0$$

$$G_U(\rho)=e^{-\rho}\rho^s\sum_{m=0}^{\infty}b_m\rho^m,\quad F_U(\rho)=e^{-\rho}\rho^s\sum_{m=0}^{\infty}a_m\rho^m$$

$$\left[\frac{d}{d\rho}+\frac{\kappa}{\rho}\right]e^{-\rho}\rho^s\sum_{m=0}^{\infty}b_m\rho^m-\left[\sqrt{\frac{\alpha_1}{\alpha_2}}+\frac{\gamma}{\rho}\right]e^{-\rho}\rho^s\sum_{m=0}^{\infty}a_m\rho^m=0$$

$$-e^{-\rho}\rho^s\sum_{m=0}^{\infty}b_m\rho^m+se^{-\rho}\rho^{s-1}\sum_{m=0}^{\infty}b_m\rho^m+e^{-\rho}\rho^s\sum_{m=0}^{\infty}mb_m\rho^{m-1}+\kappa e^{-\rho}\rho^{s-1}\sum_{m=0}^{\infty}b_m\rho^m$$

$$-\sqrt{\frac{\alpha_1}{\alpha_2}}e^{-\rho}\rho^s\sum_{m=0}^{\infty}a_m\rho^m-\gamma e^{-\rho}\rho^{s-1}\sum_{m=0}^{\infty}a_m\rho^m=0$$

$$\sum_{m=0}^{\infty}\left[-b_m - -\sqrt{\frac{\alpha_1}{\alpha_2}}a_m\right]\rho^{m+s} + \sum_{m=0}^{\infty}\left[sb_m + mb_m + \kappa b_m - \gamma a_m\right]\rho^{m+s-1} = 0$$

Again we introduce $n = m-1$ for terms in second brackets.

$$\sum_{m=0}^{\infty}\left[-b_m - -\sqrt{\frac{\alpha_1}{\alpha_2}}a_m\right]\rho^{m+s} + \sum_{m=-1}^{\infty}\left[sb_{m+1} + (m+1)b_m + \kappa b_{m+1} - \gamma a_{m+1}\right]\rho^{m+s} = 0$$

$$\left[sb_0 + \kappa b_0 - \gamma a_0\right]\rho^{s-1} + \sum_{m=0}^{\infty}\left[(s+m+\kappa+1)b_{m+1} - \gamma a_{m+1} - b_m - \sqrt{\frac{\alpha_1}{\alpha_2}}a_m\right]\rho^{m+s} = 0$$

$$(s+\kappa)b_0 - \gamma a_0 = 0 \qquad (3.23)$$

For the second terms again we introduce $q = m+1$

$$(s+q+\kappa)b_q - \gamma a_q - b_{q-1} - \sqrt{\frac{\alpha_1}{\alpha_2}}a_{q-1} = 0, \quad q \geq 1 \qquad (3.24)$$

From equations (3.21) and (3.23) we find s in terms of γ and κ.

$$(s-\kappa)a_0 = -\gamma b_0 \rightarrow \quad b_0 = \frac{(s-\kappa)}{\gamma}a_0$$

$$(s+\kappa)b_0 = \gamma a_0 \quad \rightarrow \quad (s+\kappa)\frac{\kappa - s}{\gamma}a_0 = \gamma a_0$$

$$\kappa^2 - s^2 = \gamma^2$$

$$s = \pm\sqrt{\kappa^2 - \gamma^2}$$

Since as $\rho \to 0$ at the origin, $\rho^s \to \infty$ for negative s; and $\sum_{m=0}^{\infty} \rho^{m+s}$ gets better solutions with positive s. Therefore, we take $s = \sqrt{\kappa^2 - \gamma^2}$.

We assume that at $q = n' + 1$, $b_{n'+1} = a_{n'+1} = 0$ and at $q = n'$ $a_{n'} \neq 0, b_{n'} \neq 0$; where n' is the highest value of q takes.

From equations (3.22) and (3.24) we write

$$[s + n' + 1 - \kappa]a_{n'+1} + \gamma b_{n'+1} = a_{n'} + \sqrt{\frac{\alpha_2}{\alpha_1}} b_{n'}$$

From this last equation by setting $a_{n'+1} = b_{n'+1} = 0$. We obtain

$$a_{n'} = \sqrt{\frac{\alpha_2}{\alpha_1}} b_{n'} \qquad (3.25)$$

Now with $q = n'$, we multiply equation (3.22) by α_1 and equation (3.24) by $\sqrt{\alpha_1 \alpha_2}$ and we substract them

$$\alpha_1 (s + n' - \kappa) a_{n'} + \alpha_1 \gamma b_{n'} = \alpha_1 a_{n'-1} + \sqrt{\alpha_1 \alpha_2} b_{n'-1} \qquad n' \geq 1$$

$$- \left[\sqrt{\alpha_1 \alpha_2} (s + n' + \kappa) b_{n'} - \sqrt{\alpha_1 \alpha_2} \gamma a_{n'} = \sqrt{\alpha_1 \alpha_2} b_{n'-1} + \alpha_1 a_{n'-1} \right] \qquad n' \geq 1$$

$$\left[\alpha_1 (s + n' - \kappa) + \sqrt{\alpha_1 \alpha_2} \gamma\right] a_{n'} = \left[-\alpha_1 \gamma + \sqrt{\alpha_1 \alpha_2} (s + n' + \kappa)\right] b_{n'} \qquad (3.26)$$

By substituting equations (3.25) into equation (3.26) we make the following calculations

$$\left[\alpha_1(s+n'-\kappa)+\sqrt{\alpha_1\alpha_2}\gamma\right]a_{n'}=\left[\sqrt{\alpha_1\alpha_2}(s+n'-\kappa)-\alpha_1\gamma\right]\left[-\sqrt{\frac{\alpha_1}{\alpha_2}}a_{n'}\right]$$

$$\alpha_1(s+n'-\kappa)+\sqrt{\alpha_1\alpha_2}\gamma=-\alpha_1(s+n'-\kappa)+\alpha_1\sqrt{\frac{\alpha_1}{\alpha_2}}\gamma$$

After some calculations we obtain

$$s+n'=\frac{\gamma}{2}\frac{(\alpha_1-\alpha_2)}{\sqrt{\alpha_1\alpha_2}} \tag{3.27}$$

Putting values of α_1 and α_2 we write

$$s+n'=\frac{\gamma}{2}\frac{m+E-m+E}{\sqrt{m^2-E^2}}=\frac{\gamma E}{\sqrt{m^2-E^2}}$$

Taking the square of this last equation we obtain

$$\gamma^2E^2=(s+n')^2(m^2-E^2)$$

$$\gamma^2E^2+(s+n')^2E^2=m^2(s+n')^2$$

$$E_n=\frac{m(s+n')}{\sqrt{\gamma^2+(s+n')^2}}$$

$$E_n=\frac{m(s+n')\Big/(s+n')}{\sqrt{1+(\frac{\gamma}{s+n'})^2}}$$

Where $s=\sqrt{\kappa^2-\gamma^2}=\sqrt{\left(J+\frac{1}{2}\right)^2-Z^2\alpha^2}$

then

$$E_n=\frac{m}{\sqrt{1+\frac{Z^2\gamma^2}{\left(n'+\sqrt{\left(J+\frac{1}{2}\right)^2-Z^2\gamma^2}\right)^2}}} \tag{3.28}$$

Equation (3.28) gives energy eigenvalues of hydrogen atom. E depends only on n' and $J+\frac{1}{2}=|\kappa|$.

The principal quantum number $n=n'+|\kappa|=n'+J+\frac{1}{2}$. The minimum value of n' is 0. Then we get $n>J+\frac{1}{2}$ which is at least unity.

Now we expand equation (3.28)

$$E_n=\frac{m}{\sqrt{1+\frac{Z^2\gamma^2}{\left(n'+\sqrt{\left(J+\frac{1}{2}\right)^2-Z^2\gamma^2}\right)^2}}}$$

with $n=n'+\left(J+\frac{1}{2}\right)$ $\qquad n'=n-\left(J+\frac{1}{2}\right)$

$$E_n = m\left[1+\frac{Z^2\alpha^2}{\left[n-\left(J+\frac{1}{2}\right)+\left(\left(J+\frac{1}{2}\right)^2-Z^2\alpha^2\right)^{\frac{1}{2}}\right]^{-2}}\right]^{-\frac{1}{2}} \tag{3.29}$$

$$E_n = m\left\{1-\frac{1}{2}\frac{Z^2\alpha^2}{n^2}\left(1+\left[\left(\frac{J+\frac{1}{2}}{n}\right)^2-\frac{Z^2\alpha^2}{n^2}\right]^{\frac{1}{2}}-\frac{J+\frac{1}{2}}{n}\right)^{-2}\right.$$

$$\left.+\frac{3}{8}\left(\frac{Z\alpha}{n}\right)^4\left[1+\left[\left(\frac{J+\frac{1}{2}}{n}\right)^2-\left(\frac{Z\alpha}{n}\right)^2\right]^{½}-\frac{J+\frac{1}{2}}{n}\right]^{-4}+\ldots\ldots\right\}$$

$$E_n = m\left\{1-\frac{1}{2}\frac{(Z\alpha)^2}{n^2}\left[1+\frac{J+\frac{1}{2}}{n}\left[1-\left(\frac{Z\alpha}{n}\right)^2\right]^{½}-\frac{J+\frac{1}{2}}{n}\right]^{-2}+\frac{3}{8}\frac{(Z\alpha)^2}{n^4}+\ldots\ldots\right\}$$

$$E_n = m\left\{1-\frac{1}{2}\left(\frac{Z\alpha}{n}\right)^2-\frac{1}{2}\left(\frac{Z\alpha}{n}\right)^2\left(\frac{J+\frac{1}{2}}{n}\right)\left(\frac{Z\alpha}{J+\frac{1}{2}}\right)^2+\frac{3}{8}\frac{(Z\alpha)^4}{n^4}+\ldots\ldots\right\}$$

$$E_n \approx m\left[1-\frac{1}{2}\frac{(Z\alpha)^2}{n^2}-\frac{1}{2}\frac{(Z\alpha)^4}{n^3}\left(\frac{1}{j+1/2}-\frac{3}{4n}\right)-\ldots\right] \tag{3.30}$$

$E_n = -\frac{1}{2} m \frac{Z^2\alpha^2}{n^2}$ is the energy values of hydrogen atom in non-relativistic quantum mechanics.

The ground state-energy relating to $n=1$, $J = \frac{1}{2}$ is found from equation (3.29) as

$$E_{gd} = m\left[1 + \frac{Z^2\alpha^2}{\left[1 - 1 + \sqrt{1 - Z^2\alpha^2}\right]^2}\right]^{-\frac{1}{2}}$$

$$E_{gd} = m\left[1 + \frac{Z^2\alpha^2}{1 - Z^2\alpha^2}\right]^{-\frac{1}{2}} = m\left[\frac{1 - Z^2\alpha^2 + Z^2\alpha^2}{1 - Z^2\alpha^2}\right]^{-\frac{1}{2}}$$

$$E_{gd} = m\sqrt{1 - Z^2\alpha^2} \qquad (3.31)$$

The corresponding eigenfunctions with spin-up and spin-down are

$$\psi_{n=1, j=\frac{1}{2}, \uparrow}(r,\theta,\phi) = \frac{(2mZ\alpha)^{\frac{3}{2}}}{\sqrt{4\pi}} \sqrt{\frac{1+\gamma}{2\Gamma(1+2\gamma)}} (2mZ\alpha r)^{\gamma-1} e^{-mZ\alpha r} \begin{bmatrix} 1 \\ 0 \\ \frac{i(1-\gamma)}{Z\alpha}\cos\theta \\ \frac{i(1-\gamma)}{Z\alpha}\sin\theta e^{i\theta} \end{bmatrix}$$

where $\Gamma(x) = \int_0^\infty e^{-t} t^{x-1} dt$, and $\Gamma(m) = (m-1)!$ for positive integer m and $\gamma = \sqrt{1 - Z^2\alpha^2}$. We note that $\sqrt{1 - Z^2\alpha^2} \approx 1 - \frac{Z^2\alpha^2}{2}$. In the non-relativistic limit $\gamma \to 1$ get the Schrödinger wave functions multiplied by Pauli spinors. As $r \to 0$ in the relativistic case, ψ exhibits a mild singularity of order $(2mZ\alpha r)^{-Z^2\alpha^2/2}$ and this is important at distances $r \approx \frac{1}{2mZ\alpha} e^{-2/Z^2\alpha^2}$. When $Z\alpha \geq 1$, γ imaginary. In this case there is no difference between positive and negative energy spectra so the problem has no physical interpretation.

We classify energy levels of equation (3.30) by their non-relativistic labels, that is, by the orbital angular momentum l appearing in $\psi^l_{J,m}$ and by the total J.

For $1S_{1/2}$ $n = 1$, $l=0$, $J = 1/2$ $E_{nJ} = m\sqrt{1 - Z^2\alpha^2}$,

For $2S_{1/2}$ $n = 2$, $l=0$, $J = 1/2$ $E_{nJ} = m\sqrt{\frac{1 + \sqrt{1 - Z^2\alpha^2}}{2}}$

For $2P_{1/2}$ $n = 2$, $l=1$, $J = 1/2$ $E_{nJ} = m\sqrt{\frac{1 + \sqrt{1 - Z^2\alpha^2}}{2}}$

For $2P_{3/2}$ $n = 2$, $l=1$, $J = 1/2$ $E_{nJ} = m\sqrt{1 - \frac{Z^2\alpha^2}{4}}$

As we see $2S_{1/2}$ and $2P_{1/2}$ are degenerate. The $2P_{3/2}$ state has more energy than the $2P_{1/2}$ state. The state of larger J, lies higher in energy according to equation (3.30).

These results are in better agreement with the experimental results for the hydrogen atom, than the results given by the nonrelativistic treatment.

CHAPTER 4

PREVIOUS WORK

4.1. Previous Work

When Schrödinger wrote down the non-relativistic equation, he also formulated the corresponding relativistic equation. Subsequently, the identical equation was proposed independently by Gordon (1926a, b); Fock (1926a, b); Klein (1926); Kudar (1926); de Donder and van Dungen (de Donder, 1926)

In 1928 Dirac discovered the relativistic equation that now called with his name. He overcome the difficulty of the negative probability seen in the Klein-Gordon equation. The Dirac equation describes particles of $\frac{1}{2}$ spin. Both electrons and protons have $\frac{1}{2}$ spin. It is a theoretical conjecture that all elementary particles have spin $\frac{1}{2}$. It was believed that Dirac equation is the only valid relativistic wave equation for particles with mass until Pauli and Weiskopf reinterpreted the Klein-Gordon equation as a field theory in 1934.

The observed fine structure of the levels of the hydrogen atom is in good agreement with Dirac's theory. This agreement includes the degeneracy of levels with the same j and different l except for one case, namely, the $S_{1/2}$ and $P_{1/2}$. In this case Lamb (1947) found the $2S_{1/2}$ state of hydrogen is higher than $2P_{1/2}$ state, a seperation which has been explained by radiative corrections.

In Dirac equation large and small components of the wave function are related to each other by odd operators such as α . There must be a transformation which removes large and small components in two components as in the non-relativistic Pauli (1927) theory .This problem was solved by Becker (1945) to order $\frac{v^2}{c^2}$, and exactly solved by Foldy and Wouthuysen (1950) see also Tani (1951).

CHAPTER 5

5.1 Results and Discussion

In the simple Bohr model of the hydrogen atom the velocity of the electron in the first orbit is

$$v = \frac{e}{\sqrt{4\pi\varepsilon_o mr}} = \frac{1..6\times10^{-19}C}{\sqrt{4\pi(8.85\times10^{-12}F/m)(9.1\times10^{-31}kg)(5.3\times10^{-11}m)}} = 2..2\times10^{6}m/s$$

This velocity being about 1% of the velocity of light . We need to take into account the relativistic corrections.In the Bohr model the energy of the electron in the hydrogen atom is calculated as follows .

Kinetic energy of electron is

$$K = \frac{1}{2}mv^2 = \frac{e^2}{8\pi\varepsilon_0 r_n}$$

$U=-\dfrac{e^2}{4\pi\varepsilon_0 r_n}$ is the potential energy of the nucleus-electron system

Then the total energy is

$E=K+U=-\dfrac{e^2}{8\pi\varepsilon_0 r_n}$, where $r_n=n^2a_0$

The ground energy of the hydrogen atom is

$$E = -\frac{e^2}{8\pi\varepsilon_0 a_0} = \frac{(1.6\times10^{-19}C)^2}{8\pi(8.85\times10^{-12}F/m)(5.3\times10^{-11})} = -2.2\times10^{-18}j$$

Now we turn to the equation (3.30),i.e.,

$$E_n \approx m(1-\frac{1}{2}\frac{(Z\alpha)^2}{n^2}-\frac{1}{2}\frac{(Z\alpha)^4}{n^3}\left(\frac{1}{j+\frac{1}{2}}-\frac{3}{4n}\right)-....)$$

First term is rest energy . The second term $-\frac{1}{2}mc^2\frac{(Z\alpha)^2}{n^2}$ gives non-relativisticenergy of the particle.For hydrogen atom in ground state energy is

$$-\frac{1}{2}mc^2\alpha^2=-\frac{1}{2}(9.1\times10^{-31}\ kg)(3\times10^8 m/s)^2(\frac{1}{137})^2=-2.2\times10^{-18}j$$

which is the same as calculated using Bohr model.Therefore the first relativistic

correction is the term $-\frac{1}{2}mc^2\frac{(Z\alpha)^4}{n^3}\left(\frac{1}{j+1/2}-\frac{3}{4n}\right)$ For ground state this term is $-2.91\times10^{-23}j$

This term corresponds to the spin-orbit coupling which gives rise to the fine structure . The ratio of this term to the term which gives non-relativistic energy is 10^{-5}. The experimental measurements of fine structure agree very well with the above calculated value .

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